Advanced Simulation Capability for Environmental Management

Fiscal Year 2014 Status Report

Pacific Northwest NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965

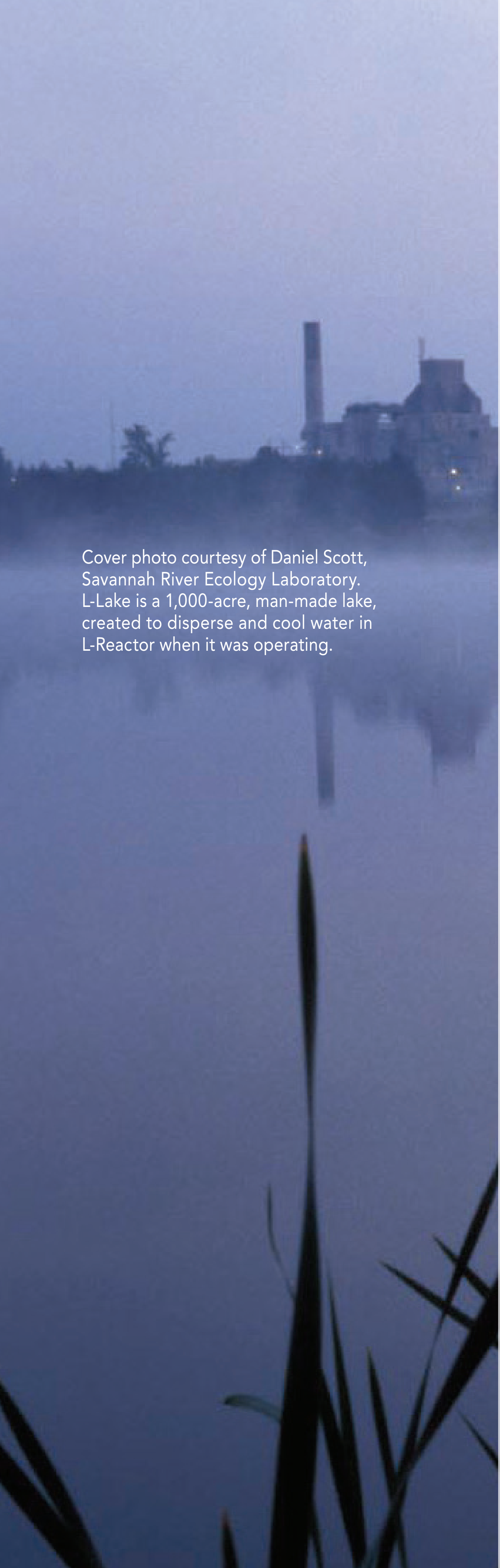
Los Alamos NATIONAL LABORATORY

BERKELEY LAB

SRNL SAVANNAH RIVER NATIONAL LABORATORY

OAK RIDGE National Laboratory

DEPARTMENT OF ENERGY UNITED STATES OF AMERICA



Cover photo courtesy of Daniel Scott, Savannah River Ecology Laboratory. L-Lake is a 1,000-acre, man-made lake, created to disperse and cool water in L-Reactor when it was operating.

Contents

Responding to the Challenge 4

Capability Development 4

References 14

Appendix: **FY14** Publications and Presentations 15

ASCEM

The Advanced Simulation Capability for Environmental Management Initiative is funded by the U.S. Department of Energy Office of Environmental Management

Message from the Office Director and Program Managers

Completing the safe cleanup of the environmental legacy brought about from five decades of nuclear weapons development and government-sponsored nuclear energy research is the mission of the U.S. Department of Energy (DOE) Office of Environmental Management (EM). Through the integration of the Advanced Simulation Capability for Environmental Management (ASCEM) Initiative and Applied Field Research Initiatives (AFRIs), the Office of Soil and Groundwater Remediation is working to deliver transformational science- and technology-based solutions to complete the EM cleanup mission. Advanced simulation capabilities are critical for cost-effective and sustainable solutions that protect human health and the environment. Through the collaborative efforts of diverse staff from the national laboratories, the ASCEM team has made excellent progress during FY 2014, including enhancements of capabilities, early deployments and use within the EM complex, and release of a research version of ASCEM to end users and sessions at EM sites for feedback and evaluation.

The ASCEM initiative will continue to make significant progress in capability enhancements, leading to release of a quality assured version in 2015 and transfer to EM sites for use. In addition, ASCEM will continue demonstration activities at the Nevada National Security Site (Pahute Mesa), Savannah River (F-Area and H-Area Tank Farm), Hanford (Waste Management Area C), and actively be seeking other site opportunities.

Kurt Gerdes
Director, Office of Soil and Groundwater Remediation
U.S. Department of Energy

Paul Dixon
ASCEM Multi-Lab Program Manager

Justin Marble
ASCEM DOE Program Manager

Responding to the Challenge

ASCEM is a state-of-the-art modeling workflow with integrated toolsets to understand and predict contaminant fate and transport in natural and engineered systems (Freedman et al. 2014). The toolsets are modular and open source and is divided into three thrust areas: Multi-Process High Performance Computing (HPC), Platform and Integrated Toolsets, and Site Applications. ASCEM is designed to facilitate integrated approaches to modeling and site characterization that enable robust and standardized assessments of performance and risk for EM cleanup and closure activities. The ASCEM toolsets were enhanced during 2014 to better accomplish modeling workflows. It is being deployed to provide technical underpinnings for a number of analyses at DOE sites. A research version of ASCEM was released to end users during several outreach sessions to solicit feedback. All of these efforts are steps toward full deployment across the EM complex.

Capability Enhancement

ASCEM provides a workflow consisting of a set of pre- and post-processing tools for translating conceptual models into numerical models. It is based on cloud computing to provide users access to high-performance computing resources. ASCEM promotes collaborative modeling through file access for multiple users on a shared server. Multiple toolsets, including model setup, calibration, sensitivity analysis, and uncertainty quantification, are available and capabilities for geostatistics, risk, and decision support are planned. Whenever appropriate, ASCEM leverages other software developments. For instance, ASCEM utilizes Velo, a software infrastructure for defining and orchestrating workflows and managing projects, content, and metadata. Another example is VisIT which is an interactive, scalable, visualization, animation and analysis tool. Significant enhancement of capabilities occurred in the Platform (Akuna) and HPC (Amanzi) thrust areas during 2014. A focused effort resulted in release of a research version of ASCEM and successful user interactions and feedback.

Akuna

The Platform Thrust added new features and streamlined workflows that increased existing capabilities within the toolsets, while maintaining tight integration among the four primary ASCEM components: Akuna, Velo, Agni, and Amanzi (see Figure 1). Key features added to the toolsets make cloud-based integrated technologies more user-accessible and augment capabilities for uncertainty and sensitivity analyses, grid generation, data imports, and visualization. The following features and capabilities were added to Akuna:

- To support the user outreach efforts, tutorials were integrated directly into the Akuna user interface (UI), and new views were created to make collaborative modeling more accessible
- Server-side job-launching capability was added, which permits end users to launch jobs through the ASCEM server rather than their client machine to overcome organizational security controls that may deny access to supercomputing resources
- An efficient visualization tool for model setup that enables faster rendering as well as the ability to create new regions was integrated into the user interface
- A visualization analysis tool based on VisIt was integrated into Akuna

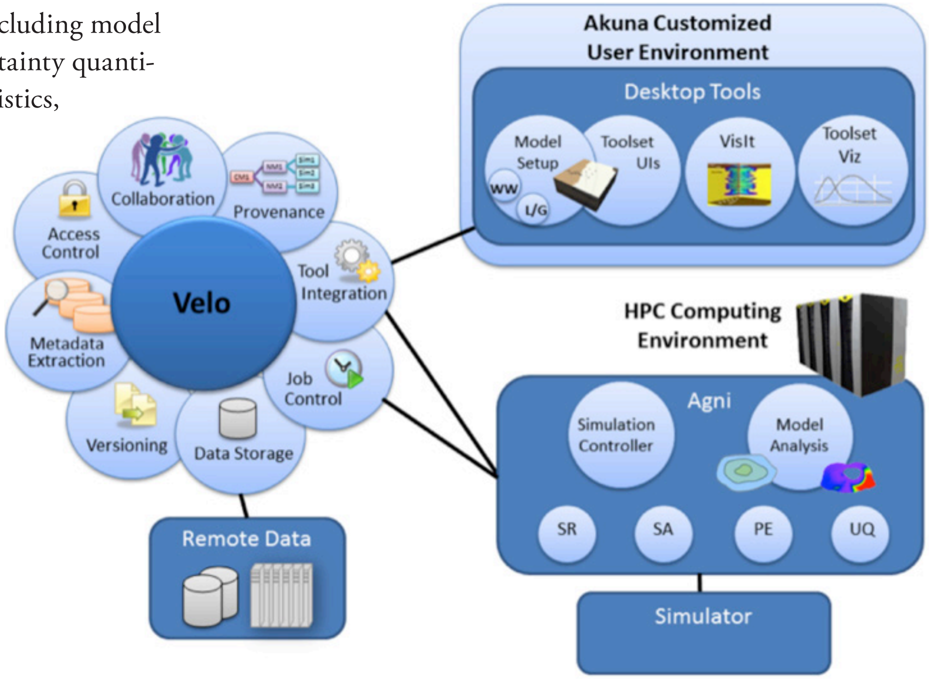


Figure 1. Overview of the four major ASCEM components: Akuna, Velo, Agni, and Amanzi.

- Additional algorithms were added the Uncertainty Quantification (UQ) and Sensitivity Analysis (SA) toolsets, as well as direct linkages to the Database Toolset through the Simulation Run (SR), SA, Parameter Estimation (PE), and UQ toolset user interfaces
- Additional Amanzi capabilities, such as linear sorption and block-structured adaptive mesh refinements were added to Akuna
- Critical infrastructure was added for integration testing with Amanzi and development of automated user interface testing.

Amanzi

The HPC Thrust balanced enhancement activities for Amanzi across improvements in performance and robustness, advances in quality assurance (QA), and enhancements to capabilities for the outreach sessions and working group collaborations. In contrast, other features of Amanzi were improved or added to support collaborations, including collaboration with working groups and outreach to the EM international programs.

- The robustness of the Akuna/Amanzi interface was enhanced and readability of the Amanzi input files was improved
- Additional mesh and region definitions were added to enable flexible and rapid construction of adaptive mesh refinement representations of cylindrical tanks with refined structural features
- Performance of lower level components of Amanzi was improved to enhance overall performance
- The capability for including layers that pinch out was added to gridding, as was support for prismatic cells that are used for gridding stacked surfaces, such as those used to capture subsurface remediation features
- A capability to output the flow field was added to support the use of a particle tracking code to simulate contaminant transport in fractured rock
- Amanzi's reactive transport capabilities were enhanced to include a unique capability for dispersion associated with non-grid-aligned flows, such as a curved streamline
- Geochemistry capabilities were enhanced with initial support for geochemistry engine (PFLOTRAN), through an interface library called Alquimia
- A linear distribution coefficient (K_d) model was implemented in Amanzi, which can be defined for each material, and decay through Amanzi's original geochemistry engine
- The Amanzi User Guide was improved and integrated with documentation generation tools to provide integrated testing and documentation tools for quality assurance
- A suite of geochemistry benchmark tests were enhanced to facilitate comparisons of unstructured and structured mesh frameworks, and testing of Amanzi with its native and Alquimia engines.

Early Site Deployments

As part of the development process, demonstrations and deployments are conducted to test and highlight the ASCEM workflow, engage end users in applications, and provide feedback to software developers. The overall approach consists of testing components and integrated capabilities at an increasing number of DOE sites and with different data sets over time. To accomplish this, the Site Applications Thrust engages end users through working groups, including the Deep Vadose Zone (DVZ) and WMA C performance assessment at the Hanford Site, waste tank performance assessment at the Savannah River Site (SRS), F Area at SRS, and the Nevada Nuclear Security Site (NNSS, formerly the Nevada Test Site). All of these deployments involve collaboration with the EM sites and co-funding.

Deep Vadose Zone Working Group

The DVZ working group is supporting performance assessment of the single-shell tank Waste Management Area C (WMA C or the 241-C Tank Farm), located on the Hanford Site's Central Plateau. Closing WMA C requires a long-term closure performance assessment evaluating the impacts on human health and the environment from residual tank and ancillary equipment wastes after retrieval and removal are complete. Under closure scenarios, the fate and transport calculations will be used to estimate concentrations at downstream locations in the groundwater and a performance or risk assessment will apply various human exposure scenarios to estimate potential future risks, including radiological dose and hazardous chemical exposure. The Hanford DVZ working group is using the ASCEM workflow to investigate the possible effects of heterogeneities on the long-term fate and transport of tank residuals, a concern that has been voiced by regulators and stakeholders. As shown in the ASCEM demonstration with BC Cribs (Freshley et al. 2012), also in the Central Plateau, heterogeneities may be an important feature influencing subsurface flow and transport. If heterogeneities are determined to have a minimal impact, the ASCEM can provide technical defensibility for the baseline conceptual model currently being used in the WMA C performance assessment. If heterogeneities are determined to have a more significant impact, the alternative conceptual model can be transferred to the contractor performing the analysis. In 2014, the DVZ working group developed grids for simulation (Figures 2a and b). Although Figure 2 shows the major stratigraphy, this grid will be used to simulate the heterogeneous distributions currently under development.

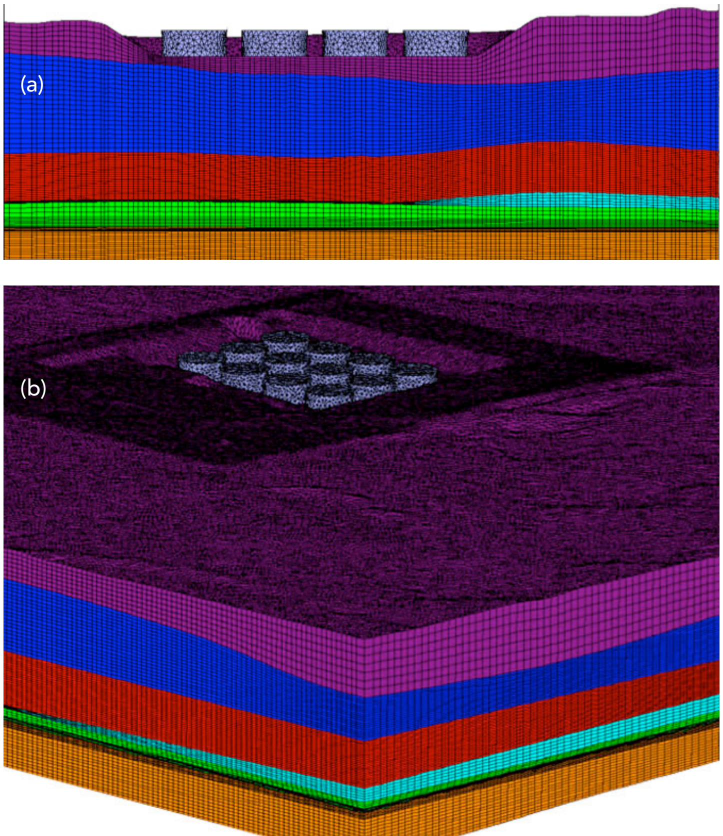


Figure 2. Unstructured grid of WMA C in a) cross-section and b) in oblique view.

Waste Tank Performance Assessment Working Group

The Waste Tank performance assessment working group is using the ASCEM toolset to address a longstanding technical concern expressed during an ongoing Nuclear Regulatory Commission (NRC) review of the H-Area Tank Farm (HTF) performance assessment (Savannah River Remediation LLC 2012) that the analysis does not address waste release from submerged and partially submerged tanks via preferential pathways (NRC 2013). The ASCEM workflow is being used to evaluate the waste tank problem by incorporating more efficient meshing capabilities, such as adaptive mesh refinement and flexible unstructured gridding, and using high-performance computing numerical algorithms and hardware. Figure 3 illustrates key features of a submerged Savannah River Type I waste tank and the simplified conceptual model.

Several meshes were generated, one based on multiple structured grid levels using adaptive mesh refinement and a second unstructured mesh that uses grid cells of variable shape and density to achieve local refinement. Flow simulations were performed on prototype two-dimensional models using structured adaptive mesh refinement and unstructured grids to assess gridding strategies and to verify model flow predictions. Figure 4 illustrates a typical flow simulation using the structured option.

The Waste Tank PA working group has defined a joint ASCEM-CBP demonstration. For the demonstration, ASCEM will be

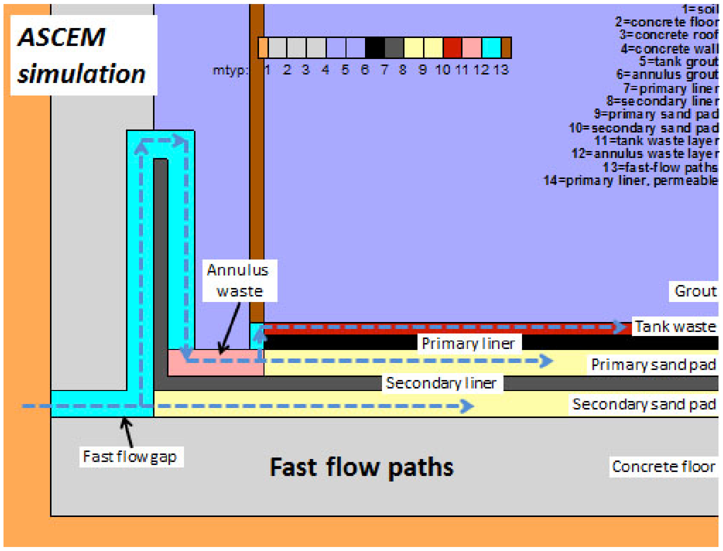


Figure 3. Geometry of the conceptual tank features and potential preferential flow paths.

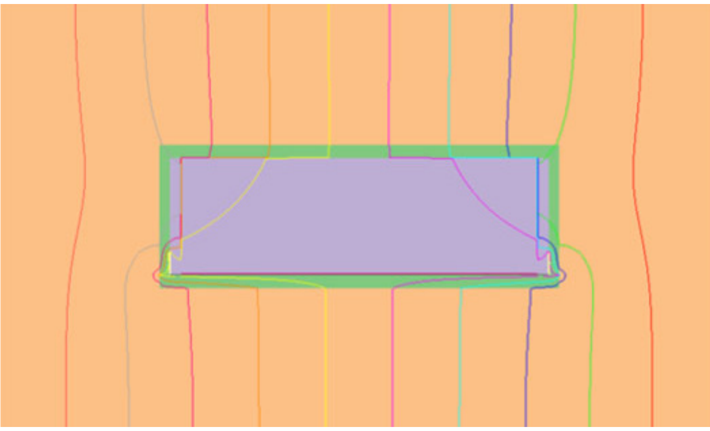


Figure 4. Simulated hydraulic head profile using structured AMR for a 2D prototype simulation.

used to simulate far-field flow conditions around a closed waste tank. The ASCEM flow field will then be used as boundary conditions for a near-field CBP simulation of contaminant leaching through cementitious materials (tank-fill grout and concrete barriers). The leach rate from the CBP near-field model will become the source term for an ASCEM simulation of far-field contaminant transport to the water table.

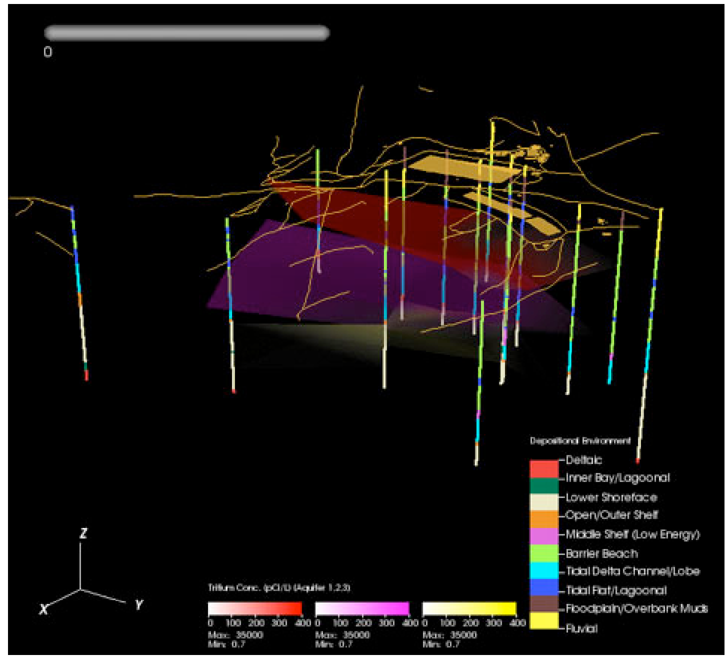


Figure 5. Three-dimensional tritium plume visualization along with surface topography, roads, building footprints, depositional facies from well logs, and a contour map of the plume for three aquifers created on their hydrostratigraphic interfaces.

Attenuation-Based Remedies for the Subsurface Working Group

The Attenuation-Based Remedies for the Subsurface (ABRS) working group focuses on demonstrating, testing, and providing drivers for capabilities development within ASCEM by implementing an integrated flow-geochemistry-transport model at the SRS F Area in South Carolina. In 2014, the SRS F Area working group supported the ABRS Applied Field Research Initiative (AFRI), also funded by the Office of Soil and Groundwater Remediation, using ASCEM. The ABRS AFRI is currently developing efficient and cost-effective approaches for long-term monitoring of sites contaminated with metals and radiological contaminants. To support these efforts, the SRS F Area working group has (1) applied the ASCEM visualization and data management toolsets to visualize the tritium and other plumes (Figure 5), (2) developed a geochemical reaction network for simulating the reactions that occurred at the site during the pH manipulation treatment, and (3) developed and implemented a three-dimensional flow and transport model to accurately represent groundwater flow and contaminant transport at the site in the presence of engineered remediation features (Figure 6).

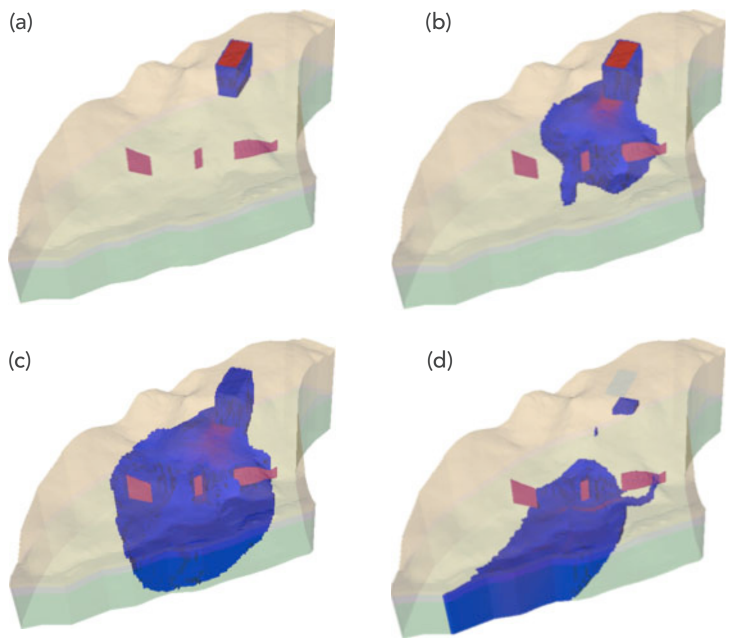


Figure 6. Non-reactive plume evolution in the 3D flow and transport model: (a) 1955, (b) 1963, (c) 1993, and (d) 2060. The blue isosurface is the plume and the red vertical structures are the barriers.

Nevada National Security Site Working Group

The ASCEM toolset is being applied to a test case that is relevant to the Underground Test Area (UGTA) at NNSS, focused on developing more detailed benchmark problems for testing the Amanzi code against analytical solutions relevant to the site. The benchmark problems entailed heterogeneous systems composed of zones with contrasting aquifer properties (Figure 7). A demonstration is being developed using new particle tracking capabilities being implemented in Amanzi to evaluate alternative conceptualizations of transport. Parameter sensitivities are being investigated using Akuna's toolset and an uncertainty analysis is being performed. As a test problem, this effort is giving UGTA staff experience implementing the ASCEM workflow on a relevant site problem.

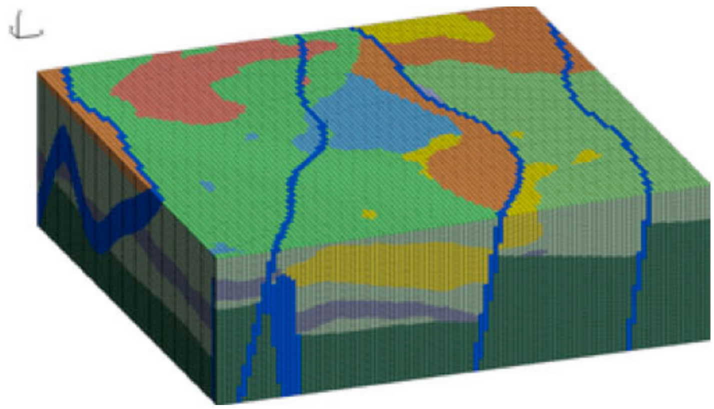


Figure 7. Numerical grid of the NNSS model domain, based on a 2014 Pahute Mesa hydrologic flow model including six fault zones.

User Release and Interactions

The ASCEM workflow and tutorials were released as a research version to an initial group of users for testing and evaluation. Executable files and the tutorial problems were made available for download through http://ascemdoe.org.

User outreach occurred through focused sessions at the Hanford Site and SRS, and through ongoing user interactions. The Hanford and SRS outreach sessions were well attended and included participants from DOE, national laboratories, and site contractors responsible for modeling and simulation. Participants provided feedback that it is useful to have the toolsets in one package, including calibration and post-processing, instead of using individual software packages and transferring data and model outputs between them.

The ASCEM project also routinely interacts with users from around the DOE complex who were not involved in the outreach or working group activities. During 2014 interactions took place with users, oversight personnel, and regulators at Hanford, Idaho, Los Alamos, Nevada, Savannah River, Portsmouth, and Paducah. Interactions continued with the Low-Level Waste Disposal Facility Federal Review Group, the EM group responsible for reviewing PAs and other documentations in support of tank closure and waste disposal activities subject to compliance with DOE Order 435.1. The ASCEM team also is engaged with the Interstate Technology and Regulatory Council, a state-led national coalition dedicated to better environmental protection through innovative technologies. These interactions provide another means to obtain input and feedback from the broader user and regulatory community.

Future Direction

During 2015, ASCEM is emphasizing deployments, increasing robustness of the current toolsets through testing, and completing quality assurance documentation for final release. The project is continuing the early deployments described in this status report, with focus on the two performance assessments at the Hanford Site and SRS. Risk and decision support toolsets are being added to complete the workflow. Quality assurance testing and documentation is a critical part of 2015 activities in order to complete an Applied-Phase Release. In 2016 and beyond, ASCEM will be deployable by EM sites, with continued support from the Office of Soil and Groundwater Remediation.

References

Freedman VL, X Chen, SA Finsterle, MD Freshley, I Gorton, LJ Gosink, E Keating, C Lansing, WAM Moeglein, CJ Murray, GSH Pau, EA Porter, S Purohit, ML Rockhold, KL Schuchardt, C Sivaramakrishnan, VV Vesselinov, and SR Waichler. 2014. "A high-performance workflow system for subsurface simulation." *Environmental Modelling & Software* 55:176-189. doi:10.1016/j.envsoft.2014.01.030

Freshley MD, S Hubbard, GP Flach, VL Freedman, DA Agarwal, BJ Andre, YJ Bott, X Chen, JA Davis, B Faybishenko, I Gorton, CJ Murray, D Moulton, JG Meyer, ML Rockhold, A Shoshani, CI Steefel, H Wainwright, and SR Waichler. 2012. *Phase II Demonstration*. PNNL-21900, ASCEM-SITE-2012-01, U.S. Department of Energy, Office of Environmental Management, Washington, D.C.

Savannah River Remediation LLC. 2012. *Performance Assessment for the H-Area Tank Farm at the Savannah River Site*. SRR-CWDA-2010-00128, Rev. 1, Aiken, South Carolina. Accessed September 24, 2014 at http://pbadupws.nrc.gov/docs/ML1304/ML13045A499.pdf.

NRC - U.S. Nuclear Regulatory Commission. 2013. *NRC Staff Request for Additional Information on the Draft Basis for Section 3116 Determination and Associated Performance Assessment for the H-Area Tank Farm at the Savannah River Site*. Washington, D.C. Accessed September 24, 2014 at http://pbadupws.nrc.gov/docs/ML1319/ML13196A133.pdf.

Appendix: FY14 Publications and Presentations

ASCEM actively participates in the technical community. The following publications and presentations documented ASCEM efforts in FY14:

- Freedman VL, X Chen, SA Finsterle, MD Freshley, I Gorton, LJ Gosink, E Keating, C Lansing, WAM Moeglein, CJ Murray, GSH Pau, EA Porter, S Purohit, ML Rockhold, KL Schuchardt, C Sivaramakrishnan, VV Vesselinov, and SR Waichler. 2014. "A high-performance workflow system for subsurface simulation." *Environmental Modelling & Software* 55:176-189. doi:10.1016/j.envsoft.2014.01.030

- Freedman VL. 2013. "A New User Environment for High-Performance Subsurface Simulation: Assessing Uncertainty in Subsurface Transport at Hanford BC Cribs." Presented by Vicky L Freedman (Invited Speaker) at *Joint Engineering & Science Seminar Series* at Washington State University, Richland, Washington, on October 18, 2013. PNNL-SA-98943.

- Freshley MD, VL Freedman, S Hubbard, H Wainwright, TD Scheibe, D Moulton, R Seitz, and P Dixon. 2014. "Advanced Simulation Capability for Environmental Management (ASCEM), A Toolset to Enable Groundwater Protection." Abstract submitted to *EPRI Groundwater Protection Workshop*, Savannah, Georgia. PNNL-SA-101901.

- Freshley MD, VL Freedman, TD Scheibe, D Moulton, P Dixon, and J Marble. 2014. "Advanced Simulation Capability for Environmental Management (ASCEM) Overview and Example Application." Presentation to the *Federal Remediation Roundtable Meeting*, Arlington, Virginia. PNNL-SA-102544.

- Freshley MD, VL Freedman, S Hubbard, H Wainwright, C Eddy-Dilek, TD Scheibe, D Moulton, P Dixon, and J Marble. 2014. "Advanced Simulation Capability for Environmental Management (ASCEM), A toolset for evaluation of complex sites." Abstract submitted to *Federal Remediation Technology Roundtable Meeting, Remediation Management of Complex Sites: Tools and Approaches*, Arlington, Virginia.

- Freshley MD, TD Scheibe, D Moulton, VL Freedman, SS Hubbard, SA Finsterle, CI Steefel, H Wainwright, GP Flach, R Seitz, P Dixon, and J Marble. 2014. "Advanced Simulation Capability for Environmental Management Initial User Release." *Waste Management Symposia*, Phoenix, Arizona, March 2-6, 2014.

- Moulton JD, CI Steefel, S Yabusaki, K Castleton, TD Scheibe, EH Keating, and VL Freedman. 2013. "Hierarchical Testing with Automated Document Generation for Amanzi (ASCEM's Subsurface Flow and Reactive Transport Simulator)." Poster presented at *AGU 2013 Fall Meeting*, December 9-13, 2013.

- Lipnikov K. 2014. "Mimetic finite difference schemes with conditional maximum principle for diffusion problems." In Springer Proceedings in Mathematics & Statistics, *Finite Volumes for Complex Applications VII - Methods and Theoretical Aspects*, Volume 1, J Fuhrmann, M Ohlberger, C Rohde (eds), Springer, pp. 373-381.

- Garimella RV, WA Perkins, MW Buksas, M Berndt, K Lipnikov, ET Coon, JD Moulton, and SL Painter. 2014. "Mesh Infrastructure for Coupled Multiprocess Geophysical Simulations." *Procedia Engineering* 82:34-45.

- Moulton JD, ET Coon, M Berndt, and RV Garimella. 2014. "Amanzi and the Arctic Terrestrial Simulator: Flexible Multiphysics Simulators for Environment and Ecosystem Applications." Poster presented at *Algorithms and Abstractions for Assembly in PDE Codes*, Sandia National Laboratories, Albuquerque, New Mexico, May 12-14, 2014.

U.S. DEPARTMENT OF ENERGY

For more information, please contact:

Paul Dixon, *ASCEM Multi-Lab Program Manager*
Los Alamos National Laboratory
Los Alamos, NM 87545
p_dixon@lanl.gov
(505) 699-1744

▶ **ascemdoe.org**

Justin Marble, *DOE Program Manager*
DOE Office of Soil and Groundwater Remediation
justin.marble@em.doe.gov
(301) 903-7210

Kurt Gerdes, *Director*
DOE Office of Soil and Groundwater Remediation
kurt.gerdes@em.doe.org
(301) 903-7289

Pacific Northwest NATIONAL LABORATORY Proudly Operated by Battelle Since 1965

Los Alamos NATIONAL LABORATORY

BERKELEY LAB

SRNL SAVANNAH RIVER NATIONAL LABORATORY

OAK RIDGE National Laboratory